Sistema de Informação para Coligir, Apresentar e Estimar Propriedades Termoquímicas

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Sumário da Apresentação

- Contextualização
- Arquitectura do Sistema
- Funcionalidades do ThermInfo:
  - Pesquisa de Compostos
  - Previsão de Propriedades:
    - ELBA
    - Direcções Futuras

Contextualização

Propriedades Termoquímicas

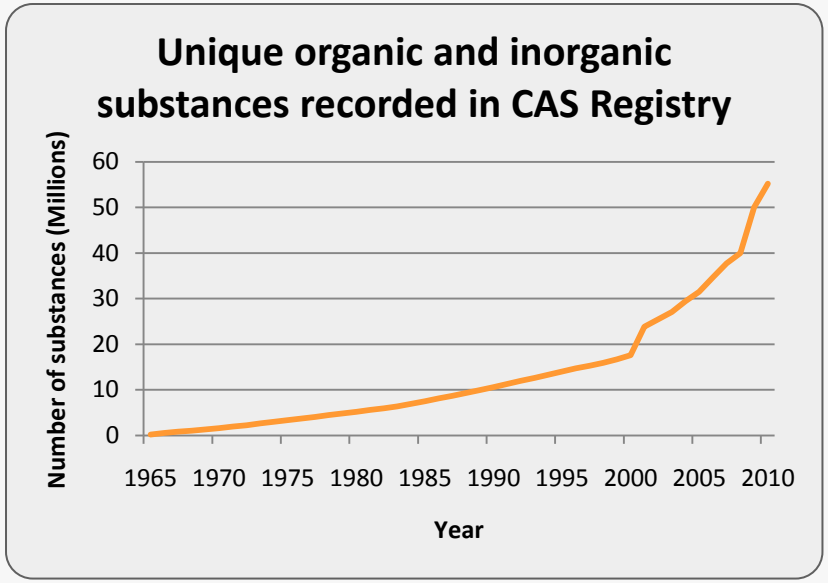
1. **Permitem estudar a natureza das ligações químicas (conteúdo energético):**
    - **Correlações entre energia, estrutura e reactividade;**
    - **Índices de perigosidade (segurança laboratorial/industrial);**
    - **Selecção de equipamento e optimização de processos industriais.**

2. **Determinação experimental complexa, morosa, cara e muitas vezes não aplicável.**

Contextualização

A química como ciência empírica

- + 55 milhões de compostos químicos
- + 12 mil novos compostos/dia



Problemas:

1. **Pesquisa de dados**
   - Livros e artigos: morosa e complexa;
   - BDs privadas: dispendiosa;
   - BDs públicas: falta de dados e/ou dados críticamente avaliados.
2. **Disponibilidade de dados sobre propriedades termoquímicas**

Arquitectura do Sistema

Fontes de Dados

Dados Compilados pelo GEM-CQB

Inserção de Dados

BD temporária

BD desactualizada

Eliminação de Dados

Actualização de Dados

Administração

Validação de Dados

Inserção de Dados

Monitorização

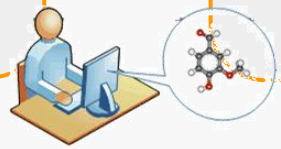
Administração

Pesquisa

Simples | Avançada | Estrutural

Resultados

Apresentação de Dados



ELBA

Simples | Estrutural

Resultados

Previsão de Propriedades

Funcionalidades do ThermInfo: Pesquisa de compostos

Search [Help]

Name | Search

Please do no

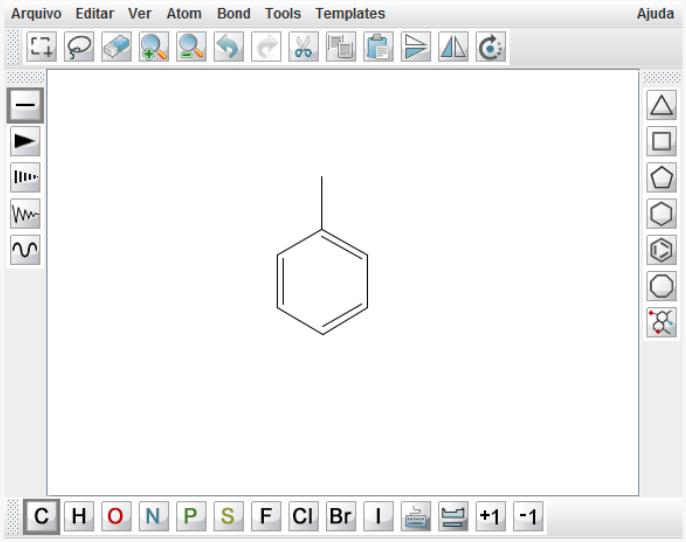
- Name
- Molecular Formula
- Molecular ID
- CAS RN
- SMILES

Security code:

[Type only **numerical characters**. Ignore letters and special characters.]

This Search Method was already used 101 times

Structural Search [Help]



Advanced Search [Help]

Compound Name: | Physical State: All

Molecular Formula: | Molecular Weight: =

[Please type Molecular Formula with atoms in **CHXNOS** (X = halogen) order]

Wildcard: **?** represents one character

SMILES: | Identical Structures

Class: All

Sub-Class: All

Family: All

Characteristic:

CH Groups	Alkane [R-H]	Alkene [R2C=CR2]	Alkyne [R-C≡C-R]	Arene [Ar-H]
CHO Groups	Alcohol [R-OH]	Ether [R-O-R]	Peroxide [R-O-O-R, R-O-OH]	Aldehyde [R(C=O)H]
	Ketone [R(C=O)R]	Carboxilic Acid [R(C=O)OH]		Ester [R(C=O)O-R]
CHN Groups	Amine [R3N]	Hydrazine [R-NH-NH-R]	Imine [R-N=R, R-N=N-R]	Nitrile/Isonitrile [R-C ≡ N, R-N$^+$ ≡ C$^-$]
CHON Groups	NOx [R3N$^+$-O$^-$, R-N=O, R-O-N=O, R-N$^+$(=O)O$^-$, R-O-N$^+$(=O)O$^-$]			Amide [R(C=O)NR2]
CHS Groups	Thiol [R-SH]	Thioether [R-S-R]	Polysulphide [R-S-S-R, R-S-SH]	Thiocarbonyl [R(C=S)R, R(C=S)H]
CHOS Groups	SOx [R2S=O, R2S(=O)2, R-O-S(=O)-O-R, R-O-S(=O)2-O-R]			
CHX Groups (X=F, Cl, Br, I)	Halogen [R-X]			
Physical	Radical	Charges	Ionic	Solvation
	Polymer			

Security code: 38J4C7

[Type only **numerical characters**. Ignore letters and special characters.]

Search

This Search Method was already used 42 times

Funcionalidades do ThermInfo: Pesquisa de compostos

You are searching for: 1,2-Dimethylbenzene .:::. Number of compounds found: 6

1. **Molecular ID:** CO01899
   Compound Name: 1,2-Dimethylbenzene
   Molecular Formula: C_8H_{10}
   CAS registry number: 95-47-6
   SMILES: Cc1ccccc1C, CC1=CC=CC=C1C
   More info: View

2. **Molecular ID:** CO01918
   Compound Name: 4-Ethyl-1,2-dimethylbenzene
   Molecular Formula: $C_{10}H_{14}$
   CAS registry number: 934-80-5
   SMILES: Cc1cc(CC)ccc1C, CC1=CC(CC)=CC=C1C
   More info: View

3. **Molecular ID:** CO01915
   Compound Name: 1-Ethyl-2,3-dimethylbenzene
   Molecular Formula: $C_{10}H_{14}$
   CAS registry number: 933-98-2
   SMILES: Cc1cccc(CC)c1C, CC1=CC=CC(CC)=C1C
   More info: View

4. **Molecular ID:** CO01999
   Compound Name: 2,3-Dimethylphenol
   Molecular Formula: $C_8H_{10}O$
   CAS registry number: 526-75-0
   SMILES: Oc1cccc(C)c1C, OC1=CC=CC(C)=C1C
   More info: View

5. **Molecular ID:** CO02008
   Compound Name: 3,4-Dimethylphenol
   Molecular Formula: $C_8H_{10}O$
   CAS registry number: 95-65-8
   SMILES: Oc1ccc(C)c(C)c1, OC1=CC=C(C)C(C)=C1
   More info: View

6. **Molecular ID:** CO02072
   Compound Name: 2,3-Dimethylbenzoic acid
   Molecular Formula: $C_9H_{10}O_2$
   CAS registry number: 603-79-2
   SMILES: O=C(O)c1cccc(C)c1C, O=C(O)C1=CC=CC(C)=C1C
   More info: View

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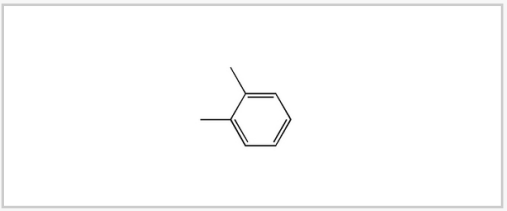
Monday, October 11, 2010

1,2-Dimethylbenzene



Structural Data

Molecular ID: CO01899 **Compound Name:** 1,2-Dimethylbenzene

Other Names: o-Xylene; o-Dimethylbenzene; o-Xylol; 1,2-Xylene; o-Methyltoluene; 2-Methyltoluene; UN 1307;

CASRN: 95-47-6 **Molecular Formula:** C_8H_{10}

Molecular Weight: 106.17 **Physical State:** Liquid

SMILES: Cc1ccccc1C, CC1=CC=CC=C1C

Unique SMILES: [c]1([c]([CH])[CH][CH][CH][CH]1)[CH3])[CH3], [C]1(=[C]([CH]=[CH][CH]=[CH]1)[CH3])[CH3]

Thermochemical Data

Standard Molar Enthalpy of Formation [kJ/mol]:

• **Crystalline Phase:**	n.a.	**Error:**	n.a.
• **Liquid Phase:**	-24.400	**Error:**	+/- 1.000
• **Gas Phase**	19.100	**Error:**	+/- 1.000

Standard Molar Enthalpy of Phase Change at 298.5 K [kJ/mol]:

• **Solid - Liquid**	n.a.	**Error:**	n.a.
• **Liquid - Gas**	43.400	**Error:**	+/- 0.000
• **Solid - Gas**	n.a.	**Error:**	n.a.

Observations: n.a.

References

1. J. B. Pedley
   Thermochemical Data and Structures of Organic Compounds, Vol. 1, 1994, 571
2. J. B. Pedley, R. D. Naylor, S. P. Kirby
   Thermochemical Data of Organic Compounds, 2nd ed., 1986, 792

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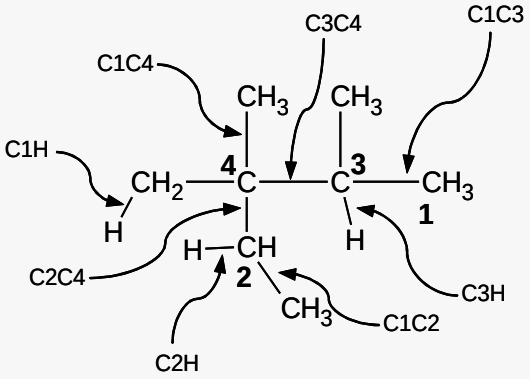
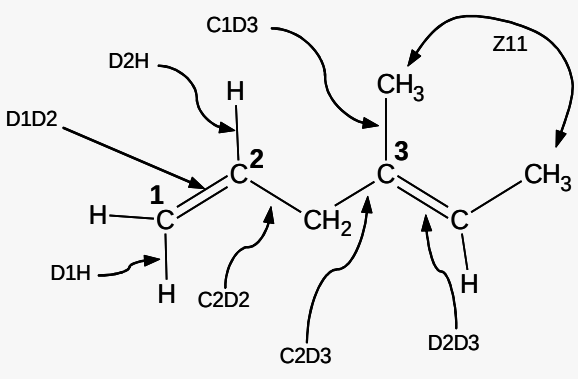
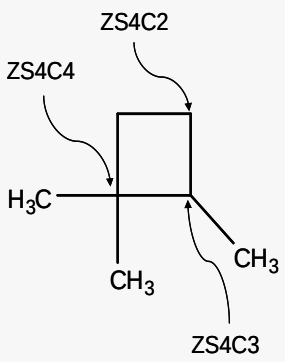
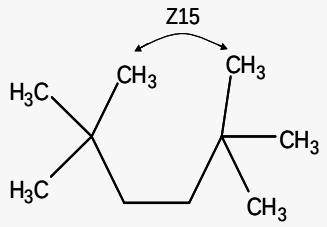
Funcionalidades do ThermInfo: ELBA

1. **Nova parametrização do método aditivo de Laidler para estimar entalpias de hidrocarbonetos:**
   - Melhores estimativas;
   - Associa um significado físico ao valor dos parâmetros;
   - Não se deixa limitar pelo elevado número de parâmetros (conjunto de 165 parâmetros para cada estado físico/mudança de estado).
2. **Extensões importantes:**
   - o tipo de ligações entre os átomos e a influência das ligações vizinhas;
   - o tipo de cadeia: linear, ramificada, e cíclica;
   - interacções não ligantes e esteroisomeria;

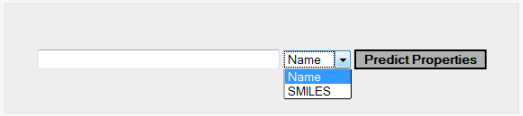


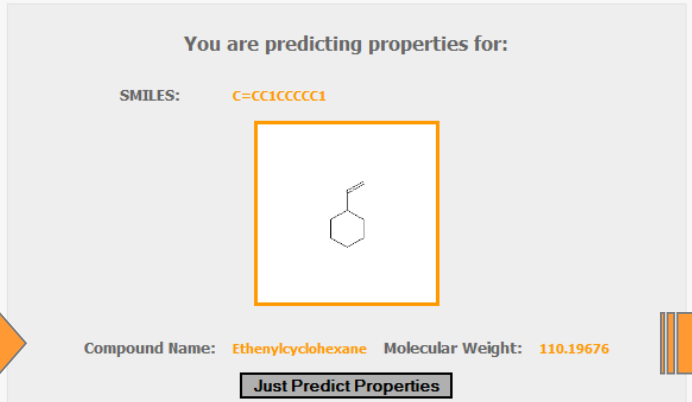


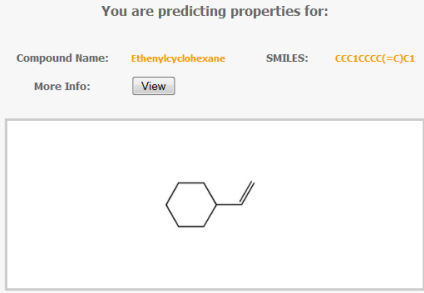


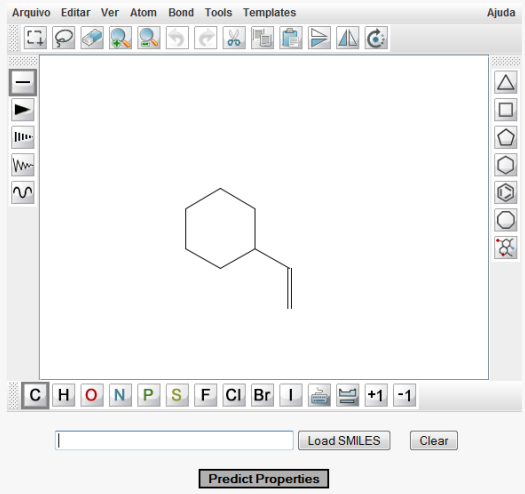


Funcionalidades do ThermInfo: ELBA



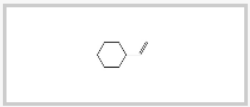




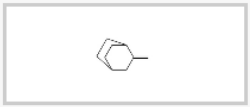


.:: Number of compounds found on the database: 2 ::.

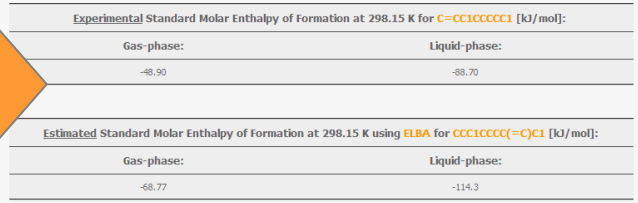
* Experimental and Estimated Properties for similar compounds found on the database: *



Molecular ID: CO01625
Compound Name: Ethenylcyclohexane
Molecular Formula: C_8H_{14}
Molecular Weight: 110.20
SMILES: C=CC1CCCCC1
Properties Prediction: View



Molecular ID: CO02671
Compound Name: 2-Methylene-bicyclo[2.2.2]octane
Molecular Formula: C_9H_{14}
Molecular Weight: 122.21
SMILES: C=C1C(CC2)CCC2C1
Properties Prediction: View



Experimental Standard Molar Enthalpy of Formation at 298.15 K for C=CC1CCCCC1 [kJ/mol]:

Gas-phase:	Liquid-phase:
-48.90	-88.70

Estimated Standard Molar Enthalpy of Formation at 298.15 K using ELBA for CCC1CCCC(=C)C1 [kJ/mol]:

Gas-phase:	Liquid-phase:
-68.77	-114.3

Set of ELBA parameters used to predict properties of CCC1CCCC(=C)C1

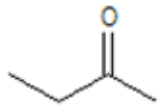
ELBA parameter	Use Frequency	Short Description [More Info]
C2C2	2	bond between two carbon atoms bonded to two carbon atoms [C-C bond for Alkanes]
C2C3	3	bond between a carbon atom bonded to two carbon atoms and a carbon atom bonded to three carbon atoms [C-C bond for Alkanes]
C1H	3	bond between a hydrogen atom and a carbon that is bonded to one carbon atom [C-H bond for Alkanes]
C3H	1	bond between a hydrogen atom and a carbon that is bonded to three carbon atoms [C-H bond for Alkanes]
C2D3	2	bond between a carbon atom bonded to two carbon atoms and a carbon atom involved in a double bond and bonded to three carbon atoms [C-C bond for Alkenes]
ZS6C2	4	secondary carbon atom in a six-carbon ring [strain parameter for cycloalkanes]
D1D3	1	double bond between a carbon atom bonded to one carbon atom and a carbon atom bonded to three carbon atoms [C-C bond for Alkenes]
ZS6D3	1	double bond connected directly to a six-carbon ring [strain parameter for cycloalkanes]
ZS6C3	1	tertiary carbon atom in a six-carbon ring [strain parameter for cycloalkanes]
C1C2	1	bond between a carbon atom bonded to one carbon atom and a carbon atom bonded to two carbon atoms [C-C bond for Alkanes]
C2H	10	bond between a hydrogen atom and a carbon that is bonded to two carbon atoms [C-H bond for Alkanes]
D1H	2	bond between a hydrogen atom and a carbon that is only involved in a double bond [C-H bond for Alkenes]
Z6	4	six-atoms ring having: one double bond in the ring, in the presence or absence of one substituent (Z6 is multiplied by two). one double bond in the ring, in the presence of two substituents (Z6 is multiplied by four). two conjugated double bonds in the ring, in the absence of one substituents (Z6 is multiplied by eight). two conjugated double bonds in the ring, in the presence of one or two substituents (Z6 is multiplied by five)[conformational parameter for cycloalkenes]

Direcções Futuras

- Estimar os parâmetros ELBA em falta;
- Implementar o ELBA para as restantes famílias de compostos químicos;
- Aplicar e comparar outros métodos de data-mining para estimar entalpias de formação;
- Aplicar estes métodos para estimar outras propriedades termoquímicas.

Direcções Futuras

1. **Utilização de matrizes de distâncias entre cada um dos átomos do composto e outros descritores estruturais(?) a definir**



A molfile for 2-butanone

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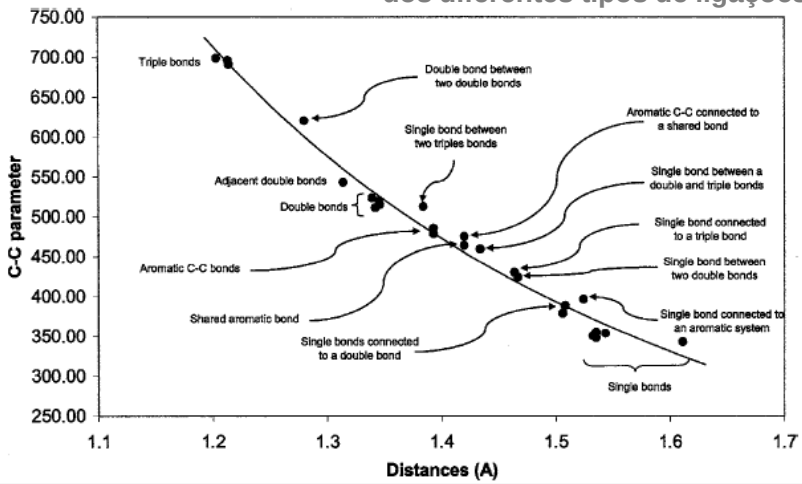
OpenBabel04121017502D
  5  4  0  0  0  0  0  0  0  0  1 V2000
    2.2994    2.0277    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.2617    0.3611    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.2994    0.9166    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.3372    0.3611    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.3750    0.9166    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  3  1  2  0
  3  2  1  0
  4  3  1  0
  5  4  1  0
M  END
```

Coordenadas x, y e z

Tabela de conectividade

Termos laidler vs distância experimental dos diferentes tipos de ligações



"The future of chemistry depends on the automated analysis of chemical knowledge, combining disparate data sources in a single resource which can be analyzed using computational techniques to assess and build on these data."

Townsend et al. (2004)

http://www.therminfo.com